

beta-Ocimene

13877-91-3 | DTXSID70274135

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.86 days

Global applicability domain: Inside

Local applicability domain index: 4.76e-01

Confidence level: 8.82e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Ethyl-2-methylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.88</div>	<div>Image not found</div> <div>2-Ethyl-p-xylene</div> <div>Measured: 12.5</div> <div>Predicted: 3.70</div>	<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div>
<div>Image not found</div> <div>1,3-Dimethyl-4-ethylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.89</div>	<div>Image not found</div> <div>1-Ethyl-2,3-dimethylbenzene</div> <div>Measured: 61.9</div> <div>Predicted: 4.15</div>	